Ising model (cont'd)

PHYS 250 (Autumn 2018) – Lecture 7

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University of Chicago

October 23, 2018

Outline

Outline of the Ising model discussion

We've already discussed a lot, and I want to remind you of those topics, their progression, and where we're going from here to make sure that we're all on the same page.

- **Lecture 5: the model iteself**
  - The general concept of the model: lattice of spins
  - Basis in thermodynamics and quantum mechanics
  - Importance of simulations methods
- **Lecture 6: computational approaches**
  - History of computational simulation methods: Monte Carlo
  - The Metropolis Monte Carlo algorithm and its assumptions (deeply related to thermodynamics)
- **Lecture 7 (Today): analytical and computational evaluation**
  - Analytical Ising model and the key numerical results
  - Concept of equilibrium and how we can define it
  - Observables in the Ising model and their calculation
- **"Lecture 8" (Tomorrow): Hands-on lab+lecture**
  - Hands-on session in CSIL 2 for developing our Ising model simulation

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Recall our discussion of statistical mechanics

We discussed that the probability distribution of an observable such as the mean energy, $\langle E \rangle$, of a system in a particular microstate μ is given by

$$\langle E \rangle = \frac{\sum_\mu E_\mu e^{-\beta E_\mu}}{\sum_\mu e^{-\beta E_\mu}} = \frac{\sum_\mu e^{-\beta E_\mu}}{Z} \tag{1}$$

where Z is the **partition function** of the system ($\beta = (k_B T)^{-1}$).

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Similarly, the variance is given by:

$$Var(E) = \langle E^2 \rangle - \langle E \rangle^2 = -\frac{\partial \langle E \rangle}{\partial \beta} = \frac{\partial^2 \ln Z}{\partial \beta^2} \tag{4}$$

Ising's analytic solution for a 1D spin lattice (I)

For a single dimension, and just $N = 2$ spins (the smallest possible Ising chain model) we can use the analytic form on the previous slide to write down Z exactly, and thus the mean energy (recall $E = -J \sum_{\langle ij \rangle} s_i s_j$) and its variance.

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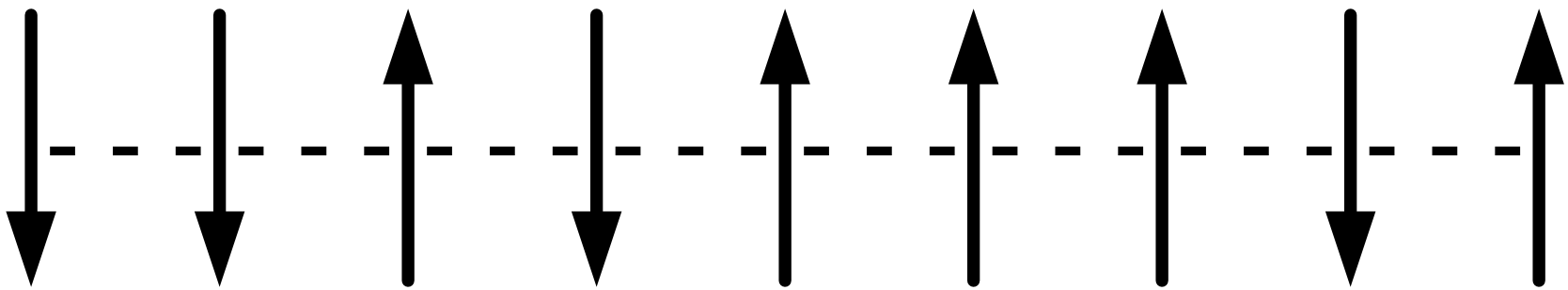

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&= (2 \cosh \beta J)^N && (15)
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(Since $Z_1 = \sum_{s_1=\pm1} 1 = 2$)

Results using Ising's analytic model (I)

With the expression for Z, we can calculate key properties of the system

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Without completing a more thorough derivation, here are three more key properties of the system:

- ***F*: Helmholtz free energy**, measures the useful work obtainable from a closed thermodynamic system at a constant T and volume. Analogous to Gibbs free energy, which does the same at constant pressure.

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Note: at constant T, Helmholtz free energy (F) is minimized at equilibrium.

(lack of) Phase transition for 1D model

The last expression for magnetization M, or magnetization per unit particle, $m = M/N$ shows a very important property

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- $M = 0$ for $H = 0$ because $\sinh x \approx x$ for small x
- For $H = 0$, $\sinh \beta H = 0$ and thus $M = 0$
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It has already been pointed out by Ising himself[4] that a linear chain of spins is not ferromagnetic. This can easily be verified by calculating the total magnetization with the help of (5) and (8):

$$M = mN \sinh C/(\sinh^2 C + e^{-4K})^{\frac{1}{2}}, \tag{10a}$$

Kramers & Wannier, 1941

Properties of the 2D Ising model

Lars Onsager, Phys. Rev. 65, 117 – Published 1 February 1944

Onsager showed in 1943 that one can solve the 2D Ising model analytically.

Solution for $\ln Z/2 = -\beta F - \ln 2$ (and allowing different J in each dimension)

$$\log(\lambda/2) = \tfrac{1}{2}\pi^{-2}\int_0^\pi\int_0^\pi \log(\cosh 2H \cosh 2H' - \sinh 2H \cos\omega - \sinh 2H' \cos\omega')d\omega d\omega'. \quad (108)$$

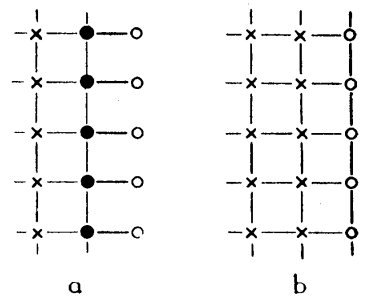

FIG. 3. Two-step extension of a two-dimensional crystal. (a) A new tier of atoms ○ is added (V_1); their configuration depends on that of atoms ● in previous marginal position. (b) Interaction energy between marginal atoms ○ is introduced (V_2), which modifies the distribution of configurations in this tier of atoms.

This leads to a relationship for the magnetization which does allow for $M \neq 0$ at $T \neq 0$, namely $T = T_c$:

$$\sinh\left(\frac{2J_1}{k_B T_c}\right)\sinh\left(\frac{2J_2}{k_B T_c}\right) = 1 \quad (24)$$

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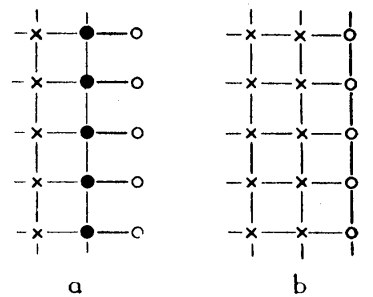

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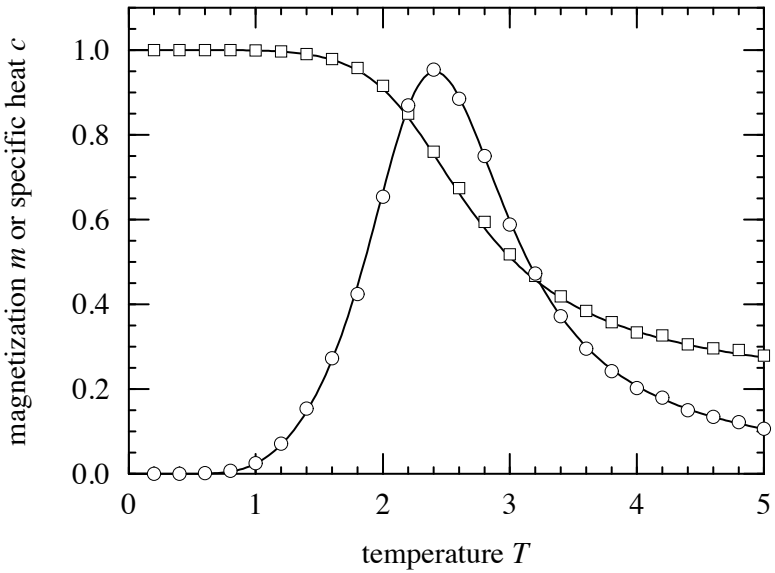
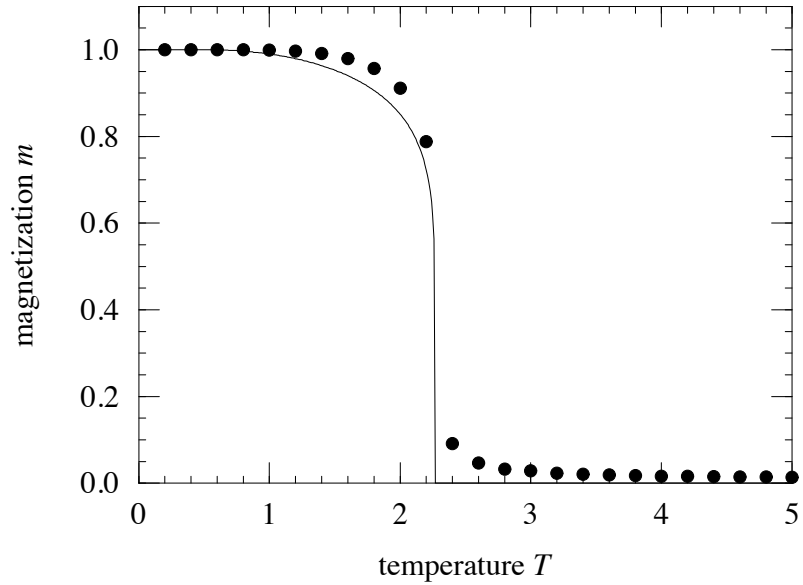
Which corresponds to

$$\frac{k_B T_c}{J} = \frac{2}{\ln(1+\sqrt{2})} \quad (25)$$

$$= 2.2692 \quad (26)$$

Simulation vs. calculations for the 2D Ising model





These results come from **two simulations (points)**, a 5×5 lattice (left) and a 100×100 lattice (right). These are compared to **analytic calculations (solid lines)**. For each simulation, a large number of Monte Carlo steps per site are run (e.g. 20,000 for the $5 \times 5 = 25 \rightarrow 500000$ steps), and averaged over the last 18000 of these to measure the magnetization and the energy. $m = M/N$ and $c = C/N$ are obtained from Eqs 21,22, and $J = k_B = 1$.

Outline

Equilibration time

In the previous slide, we stated that we needed to wait until **"the last 18000 of these to measure the magnetization"**...why is that?

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Equilibrium

In order to measure properties of the system using a simulation, we have to run our simulation for a suitably long period of time until it has come to equilibrium at the temperature we are interested in. This period is called the equilibration time τ_{eq}.

Only then can we obtain a reliable measurement of the quantity we are interested in. And then, in order to measure it's average values we must wait another suitably long period of time and average it, to evaluate the estimator of that quantity.

So many questions!

Questions you should ask yourself

- What exactly do we mean by "allowing the system to come to equilibrium"?
- How long is a "suitably long time" for it to happen?
- How do we go about measuring our quantity of interest once that happens?
- How long do we have to average over to get a result of a desired degree of accuracy?

These are very general questions which we need to consider every time we do a Monte Carlo simulation.

Discussion of equilibrium

"Equilibrium" means that the average probability of finding our system in any particular state μ is proportional to the Boltzmann weight $e^{-\beta E_\mu}$ of that state.

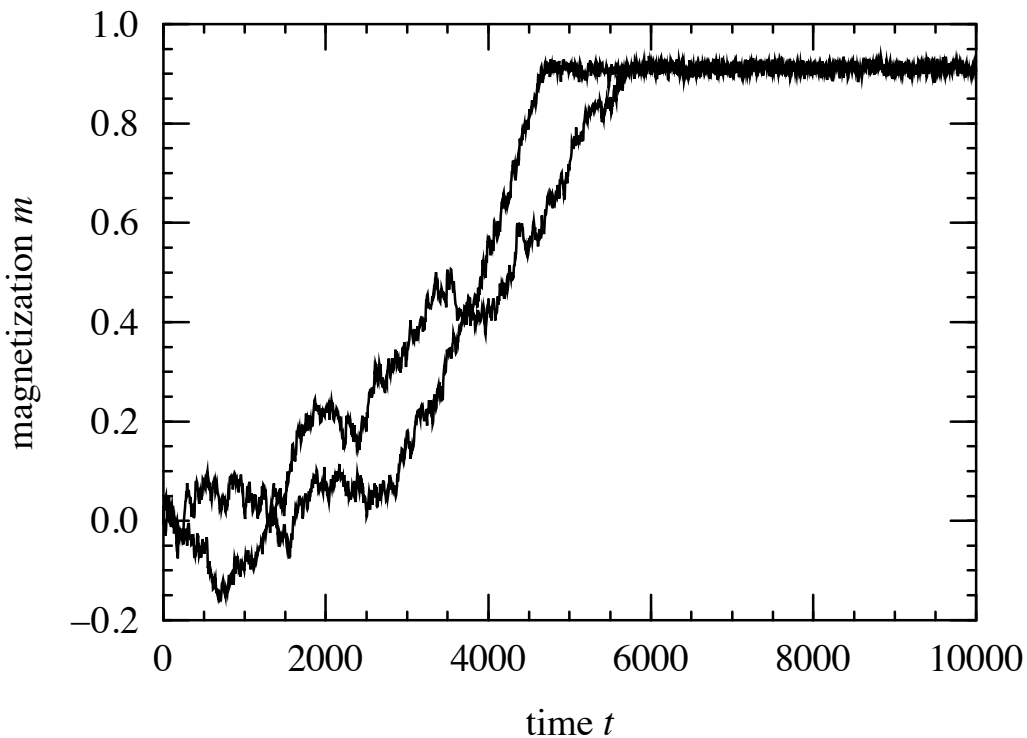
If we start our system off in a state such as the $T = 0$ (e.g. all spins aligned), and we want to perform a simulation at some finite non-zero temperature, $T \neq 0$, it will take a little time before we reach equilibrium.

A system at equilibrium spends the overwhelming majority of its time in a small subset of states in which its internal energy and other properties take a narrow range of values. This is what is "mapped out" by the temperature. To determine if the system has reached equilibrium, we could just "look at it" but this isn't very reliable.

Equilibrium in simulations

A standard approach is to plot a graph of some quantity of interest, like the magnetization per spin $m = M/N$ of the system or the energy of the system E, as a function of "time" (iterations or steps) from the start of the simulation.

Up until equilibrium, the energy and the magnetization are changing, but after equilibrium is reached, they just fluctuate around a steady average value. This is what we should measure.



Outline